

• SAFETY DATA SHEET

Version 8.4
Revision Date 01/16/2026
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SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : Alternariol-9-methyl ether-(1-methyl-d3)
solution

Product Number : 91525
Brand : Supelco

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone : +1 314 771-5765
Fax : +1 800 325-5052

1.4 Emergency telephone number

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-
527-3887 CHEMTREC (International) 24
Hours/day; 7 Days/week

SECTION 2. HAZARDS IDENTIFICATION

GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

Hazards for the product as supplied

Flammable liquids : Category 2

Acute toxicity (Oral) : Category 4

Acute toxicity (Inhalation) : Category 4

Acute toxicity (Dermal) : Category 4

Eye irritation : Category 2A

Other hazards

None known.

GHS label elements

Hazard pictograms : 

Signal word : Danger

Hazard statements : H225 Highly flammable liquid and vapour.
H302 + H312 + H332 Harmful if swallowed, in contact with skin or if inhaled.
H319 Causes serious eye irritation.

Precautionary statements : **Prevention:**
P210 Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P233 Keep container tightly closed.
P240 Ground/bond container and receiving equipment.
P241 Use explosion-proof electrical/ ventilating/ lighting equipment.
P242 Use only non-sparking tools.
P243 Take precautionary measures against static discharge.
P261 Avoid breathing mist or vapours.
P264 Wash skin thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P271 Use only outdoors or in a well-ventilated area.
P280 Wear protective gloves/ eye protection/ face protection.

Response:

P301 + P312 + P330 IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.
P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P312 IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.
P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P337 + P313 If eye irritation persists: Get medical advice/ attention.
P363 Wash contaminated clothing before reuse.

P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.

Storage:

P403 + P235 Store in a well-ventilated place. Keep cool.

Disposal:

P501 Dispose of contents/ container to an approved waste disposal plant.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Mixture
CAS-No. : Not Assigned

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
Acetonitrile	75-05-8*	$\geq 90 - \leq 100$	-

* Indicates that the identifier is a CAS No.
Actual concentration is withheld as a trade secret

SECTION 4. FIRST AID MEASURES

General advice : Show this safety data sheet to the doctor in attendance.

If inhaled : After inhalation: fresh air. If breathing stops: mouth-to-mouth breathing or artificial respiration. Oxygen if necessary. Immediately call in physician.

In case of skin contact : In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician.

In case of eye contact : After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

If swallowed : After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

Most important symptoms and effects, both acute and delayed : The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

Protection of first-aiders : For personal protection see section 8.

Notes to physician : No data available

SECTION 5. FIREFIGHTING MEASURES

Suitable extinguishing media : Water
Foam
Carbon dioxide (CO₂)
Dry powder

Unsuitable extinguishing media : For this substance/mixture no limitations of extinguishing agents are given.

Specific hazards during fire fighting : Mixture with combustible ingredients.

Pay attention to flashback.

Development of hazardous combustion gases or vapours possible in the event of fire.

Forms explosive mixtures with air at ambient temperatures.

Hazardous combustion products : Carbon oxides

Nitrogen oxides (NO_x)

Specific extinguishing methods : No data available

Further information : Remove container from danger zone and cool with water.
Suppress (knock down) gases/vapours/mists with a water spray jet.
Prevent fire extinguishing water from contaminating surface water or the ground water system.

Special protective equipment for fire-fighters : Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures	: Advice for non-emergency personnel: Do not breathe vapours, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert. Advice for emergency responders: For personal protection see section 8.
Environmental precautions	: Do not let product enter drains. Risk of explosion.
Methods and materials for containment and cleaning up	: Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

Advice on protection against fire and explosion	: Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.
Advice on safe handling	: Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.
Further information on storage conditions	: Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.
Storage class	: 3, Flammable liquids
Recommended storage temperature	: -13 - 14 °F / -25 - -10 °C
Further information on storage stability	: Store under argon.

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Components	CAS-No.	Value type (Form of exposure)	Control parameters / Permissible concentration	Basis
Acetonitrile	75-05-8	TWA	20 ppm	ACGIH
		TWA	20 ppm 34 mg/m ³	NIOSH REL
		TWA	40 ppm 70 mg/m ³	OSHA Z-1

Engineering measures : No data available

Personal protective equipment

Respiratory protection : required when vapours/aerosols are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter type: : Filter type ABEK

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Hand protection

Remarks : required

Eye protection : Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).
Safety glasses

Skin and body protection : Flame retardant antistatic protective clothing.

Hygiene measures : Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

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The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada

**MILLIPORE
SIGMA**

Appearance	: liquid
Color	: No data available
Odor	: No data available
Odor Threshold	: No data available
pH	: No data available
Melting point	: No data available
Boiling point/boiling range	: No data available
Flash point	: No data available
Evaporation rate	: No data available
Flammability (solid, gas)	: No data available
Flammability (liquids)	: No data available
Burning rate	: No data available
Upper explosion limit / Upper flammability limit	: No data available
Lower explosion limit / Lower flammability limit	: No data available
Vapor pressure	: No data available
Relative vapour density	: No data available
Relative density	: No data available
Density	: 0.786 g/cm ³
Solubility(ies)	
Water solubility	: soluble (68 °F / 20 °C)
Partition coefficient: n- octanol/water	: No data available
Autoignition temperature	: No data available
Decomposition temperature	: No data available
Viscosity, dynamic	: No data available
Viscosity, kinematic	: No data available

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Flow time : No data available

Explosive properties : No data available

Oxidizing properties : No data available

Particle characteristics
Particle size : No data available

SECTION 10. STABILITY AND REACTIVITY

Reactivity : Vapours may form explosive mixture with air.

Chemical stability : The product is chemically stable under standard ambient conditions (room temperature) .

Possibility of hazardous reactions : No data available

Conditions to avoid : Warming.

Incompatible materials : Acids
Bases
Oxidizing agents
Reducing agents
Alkali metals

Hazardous decomposition products : In the event of fire: see section 5

SECTION 11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Mixture

Acute toxicity

Acute toxicity estimate Oral - 617.01 mg/kg

(Calculation method)

Acute toxicity estimate Inhalation - 4 h - 11 mg/l - vapour(Calculation method)

Symptoms: Possible symptoms:, mucosal irritations

Acute toxicity estimate Dermal - 1,501 mg/kg

(Calculation method)

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

Remarks: Mixture causes serious eye irritation.

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

No data available

Components**Acetonitrile****Acute toxicity**

LD50 Oral - Mouse - male and female - 617 mg/kg

(OECD Test Guideline 401)

LC50 Inhalation - Mouse - male and female - 4 h - 6.022 mg/l - vapour

(OECD Test Guideline 403)

Acute toxicity estimate Dermal - 1,500 mg/kg

(Expert judgement)

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 4 h

(OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Causes serious eye irritation.

(OECD Test Guideline 405)

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Respiratory or skin sensitization

Buehler Test - Guinea pig

Result: negative

(OECD Test Guideline 406)

Germ cell mutagenicity

Test Type: Ames test

Test system: *S. typhimurium*

Result: negative

Remarks: (ECHA)

Test Type: In vitro mammalian cell gene mutation test

Test system: Chinese hamster ovary cells

Result: negative

Test Type: Mutagenicity (mammal cell test): chromosome aberration.

Test system: Chinese hamster ovary cells

Result: Positive results were obtained in some in vitro tests.

Remarks: (National Toxicology Program)

Test Type: sister chromatid exchange assay

Test system: Chinese hamster ovary cells

Result: negative

Remarks: Sister chromatid exchange

Test system: *Saccharomyces cerevisiae*

Result: positive

Remarks: Cytogenetic analysis

(ECHA)

Test Type: In vitro mammalian cell gene mutation test

Test system: Mouse lymphoma test

Result: negative

Method: OECD Test Guideline 474

Species: Mouse - male and female

Result: negative

Carcinogenicity

No evidence of carcinogenicity in animal studies.

Reproductive toxicity

Animal testing did not show any effects on fertility.

Specific target organ toxicity - single exposure

The substance or mixture is not classified as specific target organ toxicant, single exposure.

Specific target organ toxicity - repeated exposure

The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

Aspiration hazard

No aspiration toxicity classification

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity

Components:

Acetonitrile:

Toxicity to fish	: LC50 (Pimephales promelas (fathead minnow)): 1,640 mg/l Exposure time: 96 h Test Type: flow-through test Analytical monitoring: yes Remarks: (ECHA)
Toxicity to algae/aquatic plants	: NOEC (Phaeodactylum tricornutum): 400 mg/l Exposure time: 72 h Test Type: static test Analytical monitoring: yes Method: ISO 10253 GLP: yes ErC50 (Phaeodactylum tricornutum): 9,696 mg/l Exposure time: 72 h Test Type: static test Analytical monitoring: yes Method: ISO 10253 GLP: yes
Toxicity to fish (Chronic toxicity)	: NOEC (Oryzias latipes): 102 mg/l End point: mortality Exposure time: 21 d Test Type: flow-through test Analytical monitoring: yes Method: OECD Test Guideline 204 GLP: yes
Toxicity to microorganisms	: EC50 (activated sludge): > 1,000 mg/l Exposure time: 30 min Test Type: static test Method: OECD Test Guideline 209 GLP: yes

Persistence and degradability

Components:

Acetonitrile:

Biodegradability	: Inoculum: activated sludge, non-adapted Concentration: 684 mg/l Result: Readily biodegradable. Biodegradation: 70 % Exposure time: 21 d Method: OECD Test Guideline 310
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GLP: yes

Stability in water : Degradation half life (DT50): > 9,999 d pH: 7
Hydrolysis: at 25 °C
Remarks: (calculated)
Hydrolyses slowly.

Bioaccumulative potential

Components:

Acetonitrile:

Bioaccumulation : Remarks: No bioaccumulation is to be expected (log Pow <= 4).

Partition coefficient: n-octanol/water : log Pow: -0.54 (77 °F / 25 °C)
Remarks: Bioaccumulation is not expected.

Mobility in soil

Components:

Acetonitrile:

Distribution among environmental compartments : Adsorption/Soil
Koc: 16, log Koc: 1.21
Remarks: Mobile in soils (Lit.)

Stability in soil : Dissipation time: > 168 - < 672 h
Method: (calculated)
Remarks: Not expected to adsorb on soil.

Other adverse effects

Product:

Ozone-Depletion Potential : Regulation: 40 CFR Protection of Environment; Part 82 Protection of Stratospheric Ozone - CAA Section 602 Class I Substances
Remarks: This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

Components:

Acetonitrile:

Additional ecological information : Avoid release to the environment.

SECTION 13. DISPOSAL CONSIDERATIONS

Disposal methods

Waste from residues : Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

SECTION 14. TRANSPORT INFORMATION

International Regulations

IATA-DGR

UN/ID No. : UN 1648
Proper shipping name : Acetonitrile solution
Class : 3
Packing group : II
Labels : Class 3 - Flammable liquids
Packing instruction (cargo aircraft) : 364
Packing instruction (passenger aircraft) : 353

IMDG-Code

UN number : UN 1648
Proper shipping name : ACETONITRILE SOLUTION

Class : 3
Packing group : II
Labels : 3
EmS Code : F-E, S-D
Marine pollutant : no

Transport in bulk according to IMO instruments

Not applicable for product as supplied.

National Regulations

49 CFR Road

UN/ID/NA number : UN 1648
Proper shipping name : Acetonitrile SOLUTION

Class : 3
Packing group : II
Labels : Class 3 - Flammable liquids
ERG Code : 127
Marine pollutant : no

Poison Inhalation Hazard : No

Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

SECTION 15. REGULATORY INFORMATION

CERCLA Reportable Quantity

Listed substances in the product are at low enough levels to not be expected to exceed the RQ

SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

This material does not contain any components with a section 302 EHS TPQ.

SARA 313 : The following components are subject to reporting levels established by SARA Title III, Section 313:

Acetonitrile	75-05-8	>= 90 - <= 100 %
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Clean Air Act

This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B). The following chemical(s) are listed as HAP under the U.S. Clean Air Act, Section 112 (40 CFR 61):

Acetonitrile	75-05-8	>= 90 - <= 100 %
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This product does not contain any chemicals listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F).

The following chemical(s) are listed under the U.S. Clean Air Act Section 111 SOCM I Intermediate or Final VOC's (40 CFR 60.489):

Acetonitrile	75-05-8	>= 90 - <= 100 %
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Clean Water Act

This product does not contain any Hazardous Substances listed under the U.S. CleanWater Act, Section 311, Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. CleanWater Act, Section 311, Table 117.3.

This product does not contain any toxic pollutants listed under the U.S. Clean Water Act Section 307

This product does not contain any priority pollutants related to the U.S. Clean Water Act

US State Regulations

Massachusetts Right To Know

Acetonitrile	75-05-8
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Pennsylvania Right To Know

Acetonitrile	75-05-8
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Maine Chemicals of High Concern

Product does not contain any listed chemicals

Vermont Chemicals of High Concern

Product does not contain any listed chemicals

Washington Chemicals of High Concern

Product does not contain any listed chemicals

The components of this product are reported in the following inventories:

TSCA : Product contains substance(s) not listed on TSCA inventory.

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16. OTHER INFORMATION

Full text of other abbreviations

ACGIH	: USA. ACGIH Threshold Limit Values (TLV)
NIOSH REL	: USA. NIOSH Recommended Exposure Limits
OSHA Z-1	: USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
ACGIH / TWA	: 8-hour, time-weighted average
NIOSH REL / TWA	: Time-weighted average concentration for up to a 10-hour workday during a 40-hour workweek
OSHA Z-1 / TWA	: 8-hour time weighted average

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No

Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

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